

Supporting information for

Transferability of orthogonal and nonorthogonal tight binding models for aluminum clusters and nanoparticles

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Table S-1. Parameters for several TB models

method	fitting data	U_p , eV	Parameter	value
WH	2	0.0	K	0.3849
			A (eV Å C)	1020.
			B (Å $^{-1}$)	2.648
			C	0.6915
WH	2-177	0.0	K	0.4051
			A (eV Å C)	906.8
			B (Å $^{-1}$)	2.709
			C	0.2121
WH	2-177	0.0423	K	0.4096
			A (eV Å C)	877.7
			B (Å $^{-1}$)	2.7628
			C	0.003209
WH	2-177	3.0	K	0.4440
			A (eV Å C)	1102.
			B (Å $^{-1}$)	2.781
			C	0.2190
WH+SIP	2-13	0.0	K	0.4043
			A (eV Å C)	994.0
			B (Å $^{-1}$)	2.822
			C	0.02814
			β_1	4.947
			β_2	0.05968
			β_3	3.464
			R_{CO}	6.500
			Δ_{CO}	0.4748
			Δ	0.001242
			δ	1.779

Table S-1 (continued). Parameters for several TB models

WH+SOD	2–13	0.0	K	0.4112
			A (eV Å C)	855.5
			B (Å $^{-1}$)	2.743
			C	0.003864
			β_1	2.484
			β_2	0.02583
			β_3	27.15
			R_{CO}	6.500
			Δ_{CO}	0.4775
WH+SR	2–13	0.0	K	0.4316
			A (eV Å C)	599.4
			B (Å $^{-1}$)	2.312
			C	0.5748
			β_1	1.119
			β_2	0.2144
			β_3	3.645
			R_{CO}	6.500
			Δ_{CO}	0.4178

Table S-2. Parameters for several NTB models

method	fitting data	U_p , eV	Parameter	value
WH	2-177	0.0	K	1.990
			A (eV Å C)	5106.
			B (Å $^{-1}$)	3.690
			C	0.2652
			K	1.993
			A (eV Å C)	13090.
WH+SIP	2-13	0.0	B (Å $^{-1}$)	4.221
			C	0.000
			K	1.937
			A (eV Å C)	4224.
			B (Å $^{-1}$)	3.605
			C	0.4241
WH+SOD	2-13	0.0	β_1	3.084
			β_2	0.1911
			β_3	2.610
			R_{CO}	6.500
			Δ_{CO}	0.1269
			Δ	1.664
WH+SR	2-13	0.0	δ	0.7446
			K	1.872
			A (eV Å C)	3602.
			B (Å $^{-1}$)	3.523
			C	0.000
			β_1	0.3505
WH+SR	2-13	0.0	β_2	0.01178
			β_3	12.54
			R_{CO}	6.500
			Δ_{CO}	0.000
			K	1.893
			A (eV Å C)	9818.
WH+SR	2-13	0.0	B (Å $^{-1}$)	4.170
			C	0.000
			β_1	8.240
			β_2	0.5270
			β_3	0.07903
			R_{CO}	6.500
WH+SR	2-13	0.0	Δ_{CO}	0.6023

Table S-2 (continued). Parameters for several NTB models

WHXR	2	0.0	K	1.610
	2–13	0.0	K	1.770
	2–177	0.0	K	1.950
CC	2–177	0.0	A (eV Å C)	11095.
			B (Å $^{-1}$)	5.238
			C	1.128